

4-Tert-butyl-2-chlorophenyl methyl dimethylamidophosphate

Inchi:	InChI=1S/C13H21ClNO3P/c1-13(2,3)10-7-8-12(11(14)9-10)18-19(16,17-6)15(4)5/h7-9H,
InchiKey:	DHKSNLDSXLVWFF-UHFFFAOYSA-N
Formula:	C13H21ClNO3P
SMILES:	COP(=O)(Oc1ccc(C(C)(C)C)cc1Cl)N(C)C
Mol. weight [g/mol]:	305.74
CAS:	14163-82-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.35		Crippen Method
logp	4.332		Crippen Method
mccvol	230.560	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14163827&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/22-039-4/4-Tert-butyl-2-chlorophenyl-methyl-dimethylamidophosphate.pdf>

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